

University of Groningen

Erratum: Assessment of conventional density functional schemes for computing the polarizabilities and hyperpolarizabilities of conjugated oligomers

Champagne, B.; Perpète, E. A.; van Gisbergen, S. J.A.; Baerends, E. J.; Soubra-Ghaoui, C.; Robins, K. A.; Kirtman, B.; Snijders, Jaap G.

Published in:
Journal of Chemical Physics

DOI:
[10.1063/1.479106](https://doi.org/10.1063/1.479106)

IMPORTANT NOTE: You are advised to consult the publisher's version (publisher's PDF) if you wish to cite from it. Please check the document version below.

Document Version
Publisher's PDF, also known as Version of record

Publication date:
1999

[Link to publication in University of Groningen/UMCG research database](#)

Citation for published version (APA):

Champagne, B., Perpète, E. A., van Gisbergen, S. J. A., Baerends, E. J., Soubra-Ghaoui, C., Robins, K. A., Kirtman, B., & Snijders, J. G. (1999). Erratum: Assessment of conventional density functional schemes for computing the polarizabilities and hyperpolarizabilities of conjugated oligomers: An ab initio investigation of polyacetylene chains (to vol 109, art.10489, 1998). *Journal of Chemical Physics*, 110(23), 11664 - 11664. <https://doi.org/10.1063/1.479106>

Copyright

Other than for strictly personal use, it is not permitted to download or to forward/distribute the text or part of it without the consent of the author(s) and/or copyright holder(s), unless the work is under an open content license (like Creative Commons).

The publication may also be distributed here under the terms of Article 25fa of the Dutch Copyright Act, indicated by the "Taverne" license. More information can be found on the University of Groningen website: <https://www.rug.nl/library/open-access/self-archiving-pure/taverne-amendment>.

Take-down policy

If you believe that this document breaches copyright please contact us providing details, and we will remove access to the work immediately and investigate your claim.

Downloaded from the University of Groningen/UMCG research database (Pure): <http://www.rug.nl/research/portal>. For technical reasons the number of authors shown on this cover page is limited to 10 maximum.

Erratum: "Assessment of conventional density functional schemes for computing the polarizabilities and hyperpolarizabilities of conjugated oligomers: An ab initio investigation of polyacetylene chains" [J. Chem. Phys. 109, 10489 (1998)]

Ben  t Champagne, Eric A. Perp  te, Stan J. A. van Gisbergen, Evert-Jan Baerends, Jaap G. Snijders, Chirine Soubra-Ghaoui, Kathleen A. Robins, and Bernard Kirtman

Citation: J. Chem. Phys. **110**, 11664 (1999); doi: 10.1063/1.479106

View online: <https://doi.org/10.1063/1.479106>

View Table of Contents: <http://aip.scitation.org/toc/jcp/110/23>

Published by the American Institute of Physics

Articles you may be interested in

Assessment of conventional density functional schemes for computing the polarizabilities and hyperpolarizabilities of conjugated oligomers: An ab initio investigation of polyacetylene chains

The Journal of Chemical Physics **109**, 10489 (1998); 10.1063/1.477731

Density functional theory investigation of the polarizability and second hyperpolarizability of polydiacetylene and polybutatriene chains: Treatment of exact exchange and role of correlation

The Journal of Chemical Physics **125**, 194114 (2006); 10.1063/1.2388262

Density-functional theory (hyper)polarizabilities of push-pull π -conjugated systems: Treatment of exact exchange and role of correlation

The Journal of Chemical Physics **123**, 014319 (2005); 10.1063/1.1926275

PHYSICS TODAY

WHITEPAPERS

ADVANCED LIGHT CURE ADHESIVES

Take a closer look at what these environmentally friendly adhesive systems can do

READ NOW

PRESENTED BY



LETTERS TO THE EDITOR

The Letters to the Editor section is divided into three categories entitled Notes, Comments, and Errata. Letters to the Editor are limited to one and three-fourths journal pages as described in the Announcement in the 1 January 1999 issue.

ERRATA

Erratum: "Assessment of conventional density functional schemes for computing the polarizabilities and hyperpolarizabilities of conjugated oligomers: An *ab initio* investigation of polyacetylene chains" **[J. Chem. Phys. 109, 10489 (1998)]**

Benoît Champagne and Eric A. Perpète

*Laboratoire de Chimie Théorique Appliquée, Facultés Universitaires Notre-Dame de la Paix,
rue de Bruxelles 61, B-5000 Namur, Belgium*

Stan J. A. van Gisbergen and Evert-Jan Baerends

*Section Theoretical Chemistry, Vrije Universiteit, De Boelelaan 1083, 1081 HV Amsterdam,
The Netherlands*

Jaap G. Snijders

*Department of Chemical Physics, University of Groningen, Nijenborgh 4, 9747 AG Groningen,
The Netherlands*

Chirine Soubra-Ghaoui and Kathleen A. Robins

Department of Chemistry, University of Nevada, Las Vegas, Nevada 89154

Bernard Kirtman

Department of Chemistry, University of California, Santa Barbara, California 93106

[S0021-9606(99)00623-6]

The external electric field used to obtain Fig. 2 was 20×10^{-4} a.u. rather than 20×10^4 a.u.